

Operator perturbation theory in the backward Heisenberg picture

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We present a simple operator perturbation theory in the backward Heisenberg picture. Compared with the well-known Heisenberg picture, the revised picture is based on the backward time instead of the forward time. The unique feature of the uncommon picture is that the perturbation expansion becomes very simple and the famous Dyson expansion is not directly involved. Its relationship with the perturbation expansion for the density operator developed by Kubo is also discussed.

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Introduction. Consider a perturbed quantum system with the Hamiltonian

$$H(t) = H_0 + H_1(t), \quad (1)$$

where H_0 is the time-independent part and H_1 is a small time-dependent perturbation which is assumed to be switched on at initial time 0. We are interested in the following question: given an observable F that does not explicitly depend on time and its Heisenberg picture defined as

$$F^H(t) = U^\dagger(t)FU(t), \quad (2)$$

where $U(t)$ is the time evolution operator of the Hamiltonian $H(t)$ and the superscript H stands for the Heisenberg picture, can we expand the dynamic observable in the order of the perturbation based on the unperturbed system without directly resorting to the famous Dyson expansion [1]? Apparently, if the constraint was dropped, the problem would become almost trivial because of

$$U(t) = U_0(t)\mathcal{T}_+e^{(i\hbar)^{-1}\int_0^t U_0^\dagger(\tau)H_1(\tau)U_0(\tau)d\tau} \quad (3)$$

where \mathcal{T}_+ is the time-ordering operator, and $U_0(\tau) = \exp(H_0\tau/i\hbar)$ is the time-evolution operator for the unperturbed system. This question was raised when we investigated the fluctuation relations in nonequilibrium processes [2–6], and in the work we give a definite answer. We must emphasize that we aim to reinvestigate the old operator perturbation issue from a very different viewpoint and are not intended to present a method as a substitution for the Dyson expansion. In fact, we cannot even completely exclude that the same method has been in the literature.

The backward Heisenberg picture. We start by introducing a revised Heisenberg picture observable [6]

$$F^B(t, t') = U(t')F^H(t)U^\dagger(t') \quad (4)$$

with $0 \leq t' \leq t$. Because t' is the *backward* time, we call the picture as the backward Heisenberg picture and specifically indicate it by a superscript B . Obviously, if one selects $t'=0$ and t , the picture reduces to the Heisenberg and Schrödinger pictures, respectively. The equation of motion for the new defined dynamic observable $F^B(t, t')$ with respect to t' is simply

$$i\hbar\partial_{t'}F^B(t, t') = [H(t'), F^B(t, t')]. \quad (5)$$

It is worthy emphasizing that this is a terminal condition problem with $F^B(t, t)=F$ and that the Hamiltonian operator therein is indeed the Schrödinger picture, which is significantly different from the standard Heisenberg equation of motion,

$$i\hbar\partial_tF^H(t) = -[H^H(t), F^H(t)]. \quad (6)$$

with the initial condition $F^H(0) = F$. The careful reader may notice that Eq. (5) is almost same with the equation of motion for the density matrix $\rho(t)$ except that t' here is in place of the forward time t , which is not accidental because of

$$\partial_{t'}\text{Tr}\{F^B(t, t')\rho(t')\} = 0. \quad (7)$$

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The expectation value $\langle F \rangle(t)$ of the operator at time t in the picture is

$$\text{Tr}\{F\rho(t)\} = \text{Tr}\{F^H(t)\rho_0\} = \text{Tr}\{F^B(t,0)\rho_0\}, \quad (8)$$

where ρ_0 is the initial density operator that may be a pure or mixed state. To illustrate the uncommon picture, we calculate the position and momentum's backward Heisenberg pictures for a one-dimensional harmonic oscillator with a Hamiltonian $H = p^2/2m + m\omega^2 x^2/2$. Because the system is time-independent and one may easily find their equations given by

$$\partial_{t'} x(t, t') = -p(t, t')/m, \quad (9)$$

$$\partial_{t'} p(t, t') = m\omega^2 x(t, t'). \quad (10)$$

For simplicity in notations, we did not write the superscript B out explicitly. Solving both equations with the terminal conditions $x(t, t) = x$ and $p(t, t) = p$, we obtain

$$x(t, t') = [x \sin \omega t - \frac{p}{m\omega} \cos \omega t] \sin \omega t' + [x \cos \omega t + \frac{p}{m\omega} \cos \omega t] \cos \omega t', \quad (11)$$

$$p(t, t') = -[m\omega x \sin \omega t - p \cos \omega t] \cos \omega t' + [m\omega x \cos \omega t + p \cos \omega t] \sin \omega t'. \quad (12)$$

Letting $t' = 0$, the above solutions reduce to those directly calculated in the Heisenberg picture [7]. In fact, if the Hamiltonian does not depend on time, the backward Heisenberg picture (4) could not possibly show any distinctive features compared with the standard Heisenberg picture because of obvious

$$F^B(t, t') = F^H(t - t'). \quad (13)$$

Operator's perturbation. Now we turn our attention to the perturbation case (1). Substituting the perturbation expansion

$$F^B(t, t') = F_0^B(t, t') + F_1^B(t, t') + F_2^B(t, t') + \dots \quad (14)$$

into the equation of motion (5) and comparing its both sides order by order, we find

$$\begin{cases} i\hbar \partial_{t'} F_0^B(t, t') = [H_0, F_0^B(t, t')] \\ F_0^B(t, t) = F, \end{cases} \quad (15)$$

$$\begin{cases} i\hbar \partial_{t'} F_1^B(t, t') = [H_0, F_1^B(t, t')] + [H_1(t'), F_0^B(t, t'),] \\ F_1^B(t, t) = 0, \end{cases} \quad (16)$$

$$\begin{cases} i\hbar \partial_{t'} F_2^B(t, t') = [H_0, F_2^B(t, t')] + [H_1(t'), F_1^B(t, t')] \\ F_2^B(t, t) = 0, \\ \dots \end{cases} \quad (17)$$

Their formal solutions are

$$F_0^B(t, t') = U_0(t') F_0^H(t) U_0^\dagger(t') = F_0^H(t - t'), \quad (18)$$

$$F_1^B(t, t') = -(i\hbar)^{-1} U_0(t') \int_{t'}^t U_0^\dagger(\tau') [H_1(\tau'), F_0^B(t, \tau')] U_0(\tau') d\tau' U_0^\dagger(\tau'), \quad (19)$$

$$F_2^B(t, t') = -(i\hbar)^{-1} U_0(t') \int_{t'}^t U_0^\dagger(\tau') [H_1(\tau'), F_1^B(t, \tau')] U_0(\tau') d\tau' U_0^\dagger(\tau'), \quad (20)$$

...

respectively. The simplicity of Eqs. (15)-(17) contrasts sharply with the complexity of the perturbation equations for the Heisenberg picture observable

$$F^H(t) = F_0^H(t) + F_1^H(t) + F_2^H(t) + \dots, \quad (21)$$

each term on the right hand side of which satisfies

$$\begin{cases} i\hbar\partial_t F_0^H(t) = -[H_0, F_0^H(t)] \\ F_0^H(0) = F, \end{cases} \quad (22)$$

$$\begin{cases} i\hbar\partial_t F_1^H(t) = -[H_0, F_1^H(t)] - [(H_1)_0^H(t) + (i\hbar)^{-1} \int_0^t [H_0, (H_1)_0^H(\tau)] d\tau, F_0^H(t)] \\ F_1^H(0) = 0, \end{cases} \quad (23)$$

$$\begin{cases} i\hbar\partial_t F_2^H(t) = -[H_0, F_2^H(t)] - [(H_1)_0^H(t) + (i\hbar)^{-1} \int_0^t [H_0, (H_1)_0^H(\tau)] d\tau, F_1^H(t)] \\ \quad - [(i\hbar)^{-2} [\int_0^t \int_0^{\tau'} (H_1)_0^H(\tau') (H_1)_0^H(\tau'') d\tau' d\tau'', H_0]_+ - (i\hbar)^{-1} [\int_0^t (H_1)_0^H(\tau) d\tau, (H_1)_0^H(t)] \\ \quad - (i\hbar)^{-2} \int_0^t (H_1)_0^H(\tau') d\tau' H_0 \int_0^t (H_1)_0^H(\tau'') d\tau'', F_0^H(t)] \\ F_2^H(0) = 0, \\ \dots, \end{cases} \quad (24)$$

respectively, where $[\cdot, \cdot]_+$ denotes an anticommutator. We expand them until the second order, because the evolution of the n -th order $F_n^H(t)$ depends on all orders from 0 to n , and the calculations of these coefficients become considerably tedious as the order increases. However, we must point out that the relation (8) has imposed conditions

$$F_n^H(t) = F_n^B(t, 0) \quad (n = 0, 1, 2, \dots). \quad (25)$$

In the Schrödinger picture, Kubo has developed a method to evaluate the perturbation expansion for the density matrix

$$\rho(t) = \rho_0 + \rho_1(t) + \rho_2(t) + \dots \quad (26)$$

on the basis of its equation of motion in 1957, which does not depend on the Dyson expansion as well [8]. One may see that our calculation above is highly analogous to his method. Particularly, Eq. (8) has indicated

$$\text{Tr}\{\rho_n(t)F\} = \text{Tr}\{F_n^B(t, 0)\rho_0\}. \quad (27)$$

It is interesting to concretely calculate how these identities arise using the solutions (18)-(20). We use the first three order terms ($n = 0, 1, 2$) as examples. The identity with zero order is obviously trivial. For the first and second order terms, we have

$$\begin{aligned} & \text{Tr}\{F_1^B(t, 0)\rho_0\} \\ &= -(i\hbar)^{-1} \int_0^t \text{Tr}\{[H_1(\tau'), F_0^H(t - \tau')]\rho_0\} d\tau' \\ &= (i\hbar)^{-1} \int_0^t \text{Tr}\{[H_1(\tau'), \rho_0]F_0^H(t - \tau')\} d\tau' \\ &= \text{Tr}\{(i\hbar)^{-1} \int_0^t U_0(t - \tau') [H_1(\tau'), \rho_0] U_0^\dagger(t - \tau') d\tau' F\}, \end{aligned} \quad (28)$$

and

$$\begin{aligned} & \text{Tr}\{F_2^B(t, 0)\rho_0\} \\ &= (i\hbar)^{-2} \int_0^t \int_{\tau'}^t \text{Tr}\{U_0^\dagger(\tau') [H_1(\tau'), U_0(\tau' - \tau'') [H_1(\tau''), F_0^H(\tau'' - t)] U_0^\dagger(\tau' - \tau'')] U_0(\tau') \rho_0\} d\tau' d\tau'' \\ &= (i\hbar)^{-2} \int_0^t \int_0^{\tau'} \text{Tr}\{U_0^\dagger(\tau'') [H_1(\tau''), U_0(\tau'' - \tau') [H_1(\tau'), F_0^H(\tau' - t)] U_0^\dagger(\tau'' - \tau')\} U_0(\tau'') \rho_0\} d\tau' d\tau'' \\ &= \text{Tr}\{(i\hbar)^{-2} \int_0^t \int_0^{\tau'} U_0(t - \tau') [H_1(\tau'), U_0(\tau' - \tau'') [H_1(\tau''), \rho_0] U^\dagger(\tau' - \tau'')] U_0^\dagger(t - \tau') d\tau' d\tau'' F\}, \end{aligned} \quad (29)$$

respectively. Two simple formulas $\text{Tr}\{[A, B]C\} = \text{Tr}\{[B, C]A\}$ and $\text{Tr}\{[A, [B, C]]D\} = \text{Tr}\{[B, [A, D]]C\}$ are used in the derivations. We immediately find that the integral terms before the operator F in the last equalities of these equations are just $\rho_1(t)$ and $\rho_2(t)$, respectively [8, 9].

Conclusion. we give a simple operator perturbation theory in the backward Heisenberg picture. Its extension of the classical mechanical systems is straightforward.

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